



# Improvements to the CAMx Photochemical Model for Winter Ozone

**Chris Emery and Greg Yarwood**  
**Air Quality in Utah: Science for Solutions II**

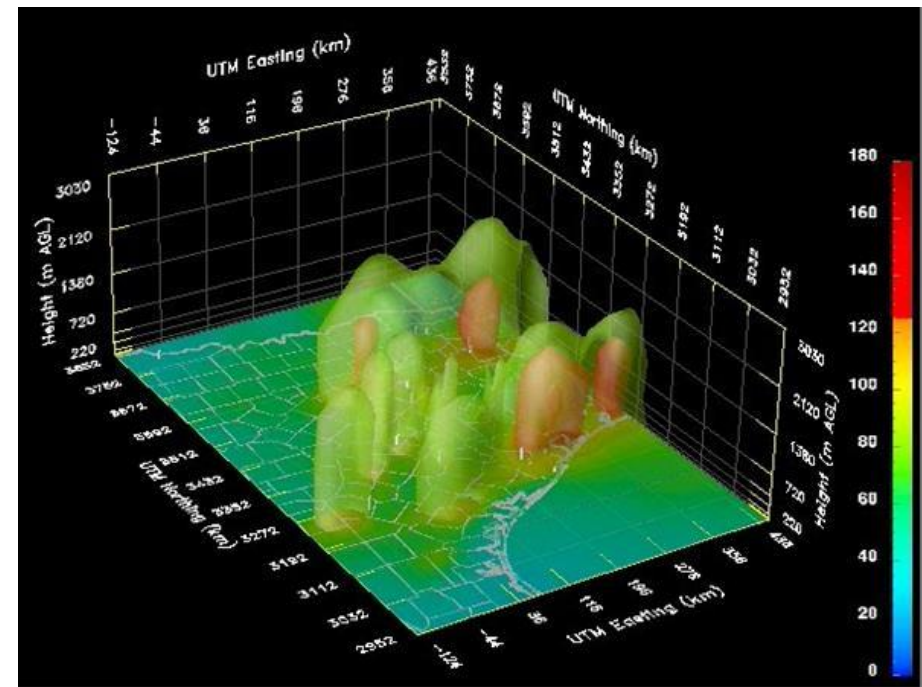
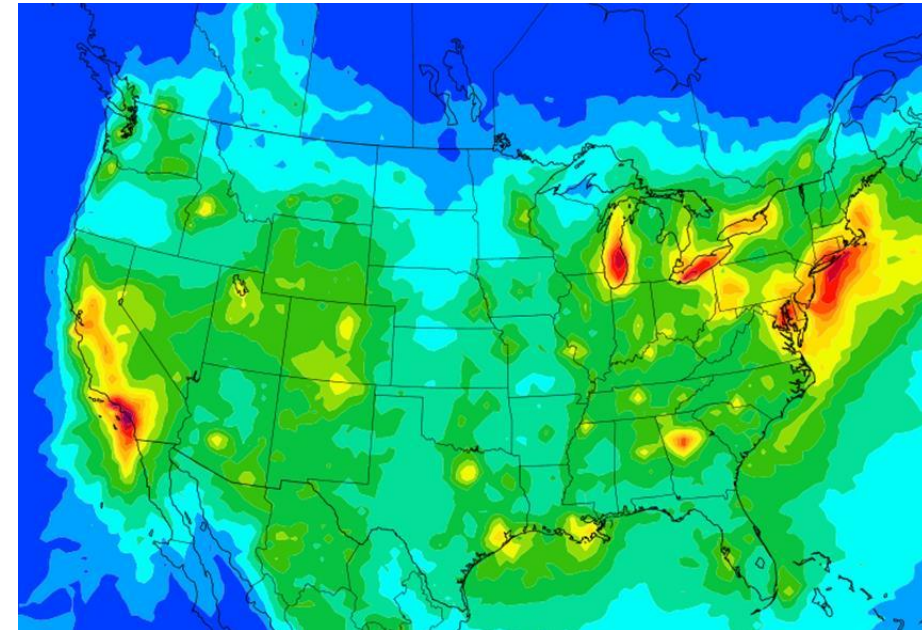
**July 28, 2015**

# ACKNOWLEDGEMENTS

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  - Patrick Barickman, Lance Avey, Kiera Harper
- Input from EPA Region 8
  - Gail Tonnesen
- Contributions from our technical staff
  - Bonyoung Koo, Jaegun Jung, Wei Chun Hsieh

# WHAT IS CAMx?

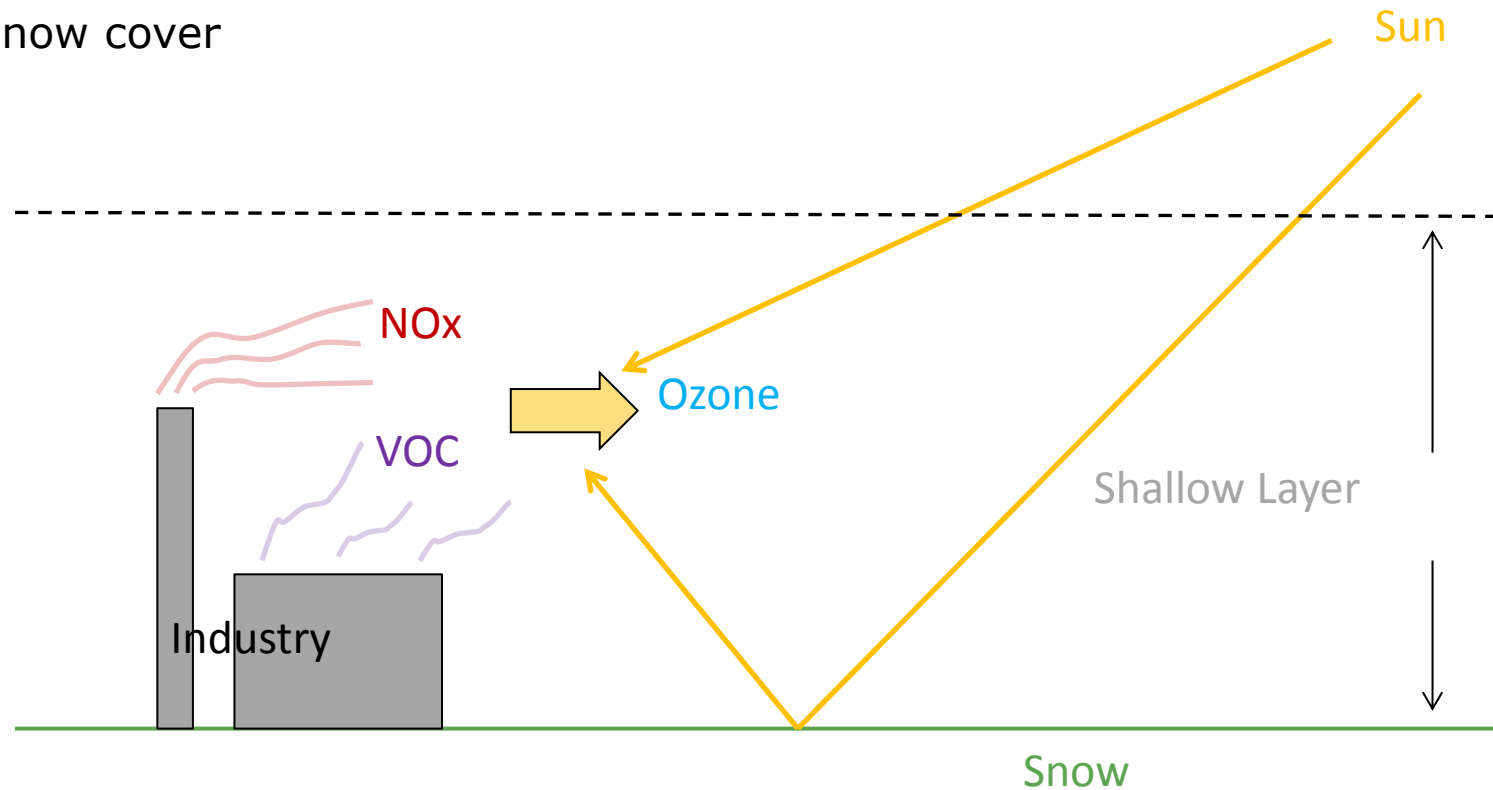
- A three-dimensional photochemical grid model
  - It's like a weather prediction model, BUT:
  - It simulates the movement and chemical evolution of pollutants through the atmosphere
- Such models help us:
  - Explain observed conditions
  - Understand complex processes
  - Identify source culpability
  - Investigate mitigation strategies
- CAMx needs many types of “big” data
  - Emissions, meteorology, surface characteristics, etc.





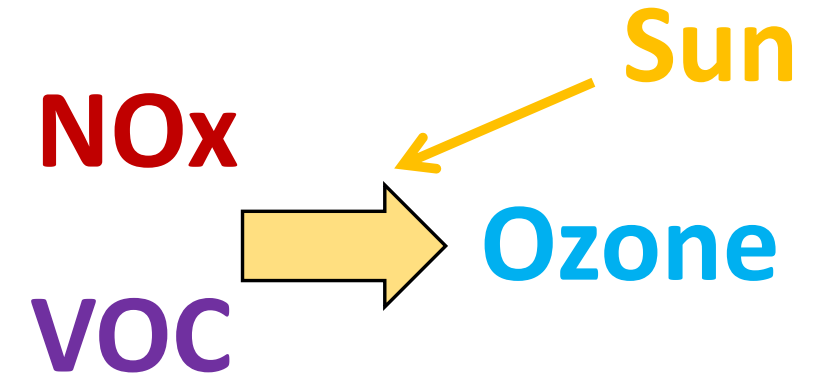
# PROJECT PURPOSE

- This project looks to improve on two pieces of the difficult wintertime ozone modeling puzzle
  - 1) Atmospheric chemistry for western Oil & Gas basin conditions
  - 2) Treatment of snow cover

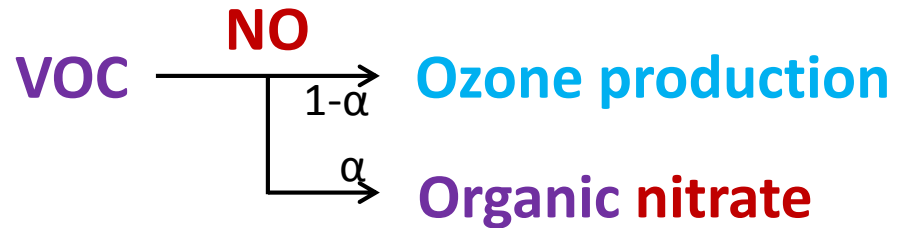


# ARE CHEMISTRY CHANGES NEEDED FOR WINTER OZONE?

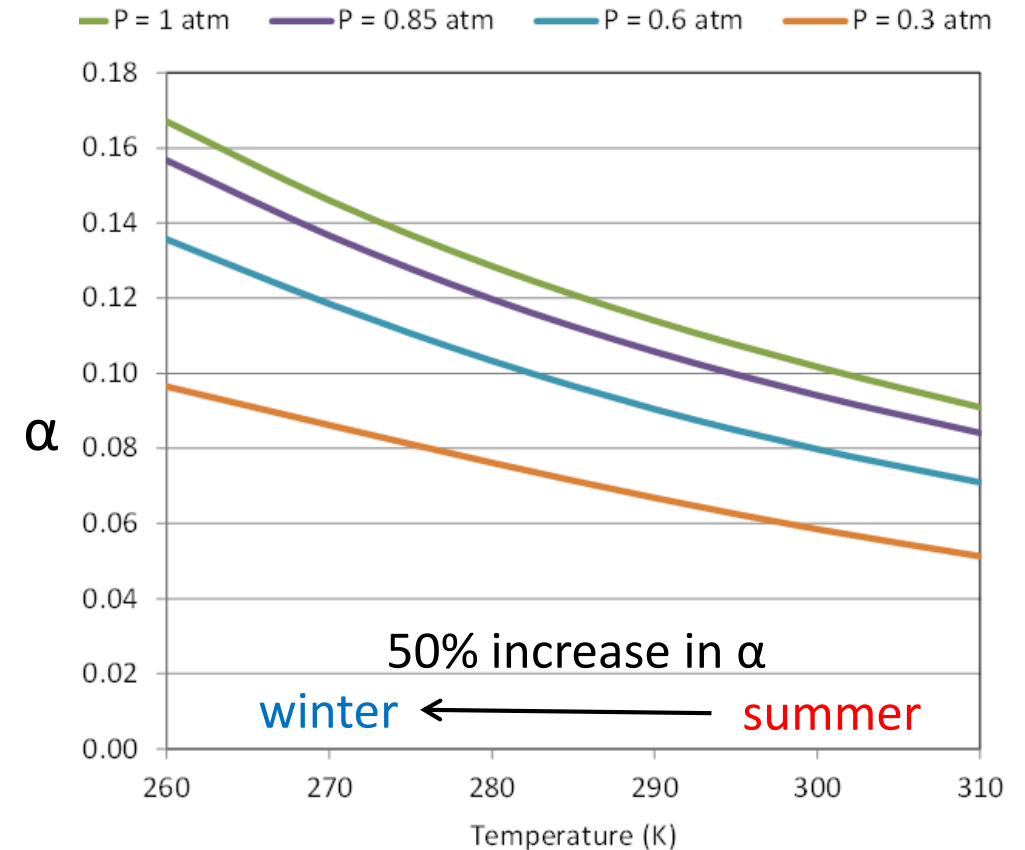
- Photolytic effect of sunlight
  - Little variation with temperature
- Chemistry of NO<sub>x</sub> and similar molecules
  - Cold conditions are understood
  - NO<sub>x</sub> chemistry is important for ozone from surface through stratosphere
- Chemistry of VOC
  - Models developed for summer ozone
  - There is potential for improvement
  - Focus on the most abundant VOCs in western US O&G basins: Alkanes



# ALKANE CHEMISTRY



- Fraction ( $\alpha$ ) of organic nitrate formed depends on temperature and pressure (altitude)
  - But models hold  $\alpha$  constant
  - Including this dependency should improve winter chemistry modeling
  - Important for O&G basin conditions
- Dynamic branching ratio added to CB6(r3)



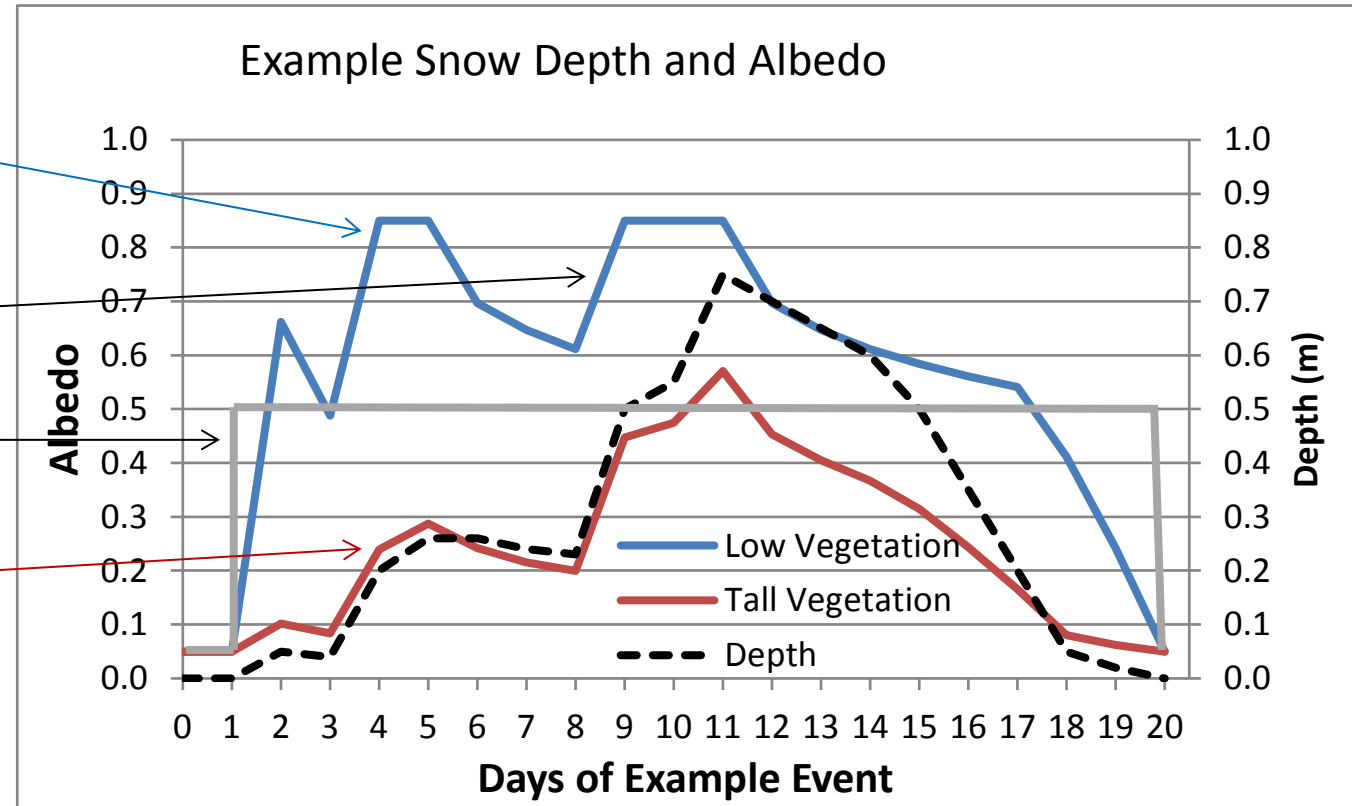
# IMPROVEMENTS FOR SNOW ALBEDO

Low vegetation covered  
faster/completely, maximizing snow  
albedo

New snowfall increases snow depth  
and “freshens” the albedo

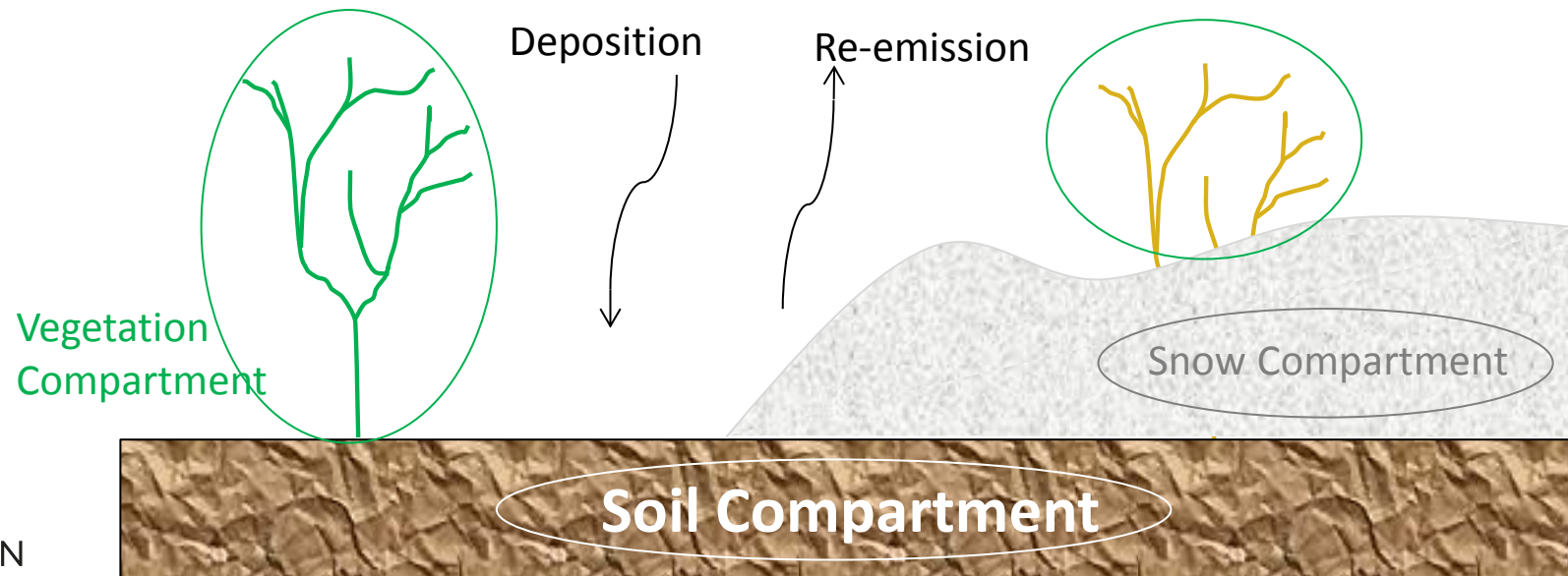
Original albedo assumption

Tall vegetation covered  
slower/incompletely, minimizing  
snow albedo



# SURFACE CHEMISTRY UPDATE

- Optional model component:
  - Two-way transfer between atmosphere and surface system
  - Chemical interactions among deposited material form products that re-emit
- Updated to include snow with soil and vegetation compartments
- Do models need to account for snow surface-atmosphere chemistry interaction?
  - May be an important contributor to atmospheric chemistry

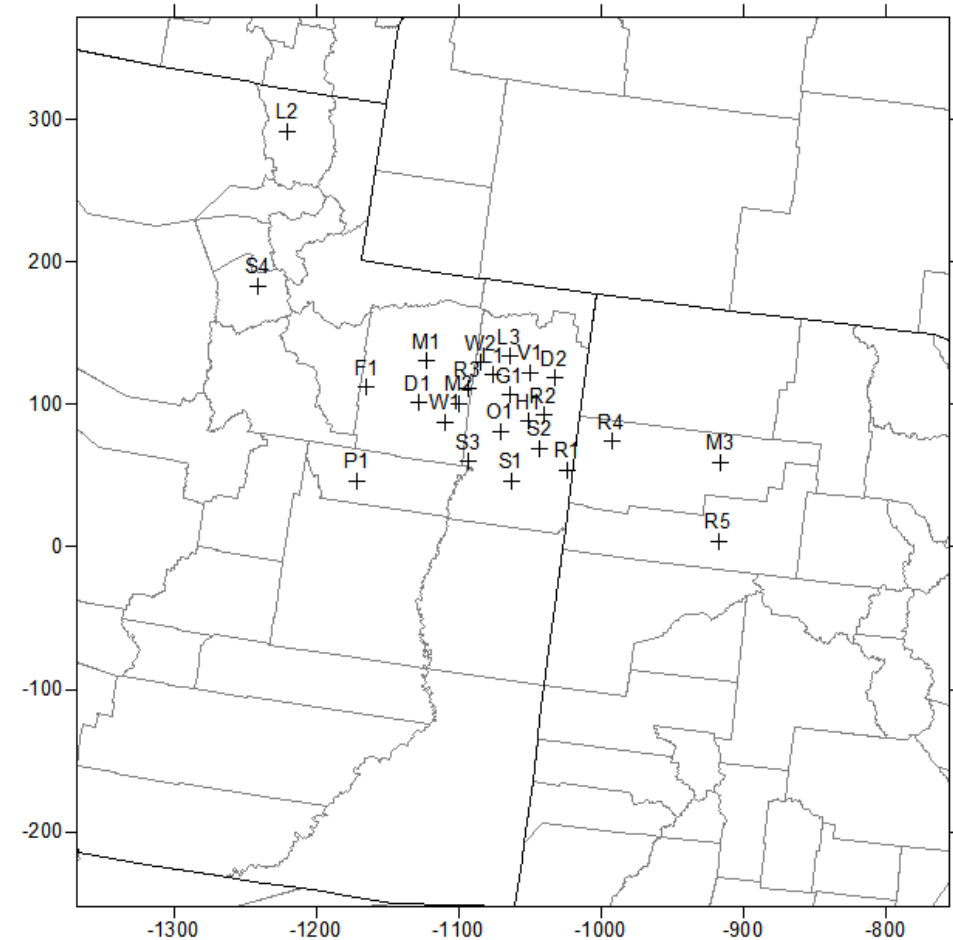




# EVALUATION IN UINTA BASIN

- **Model:**
  - CAMx v6.1 with snow/chemistry updates
- **Domain:**
  - UDAQ 4-km grid over eastern Utah
  - February 1-7, 2013 (during UBOS)
- **Datasets:**
  - UofU-derived meteorology
  - (Initial) Older UDAQ-derived emissions
  - (Latest) NEIv2/UDAQ-derived emissions
  - Boundary conditions from a global model
  - NOAA/UBOS 2013 measurements

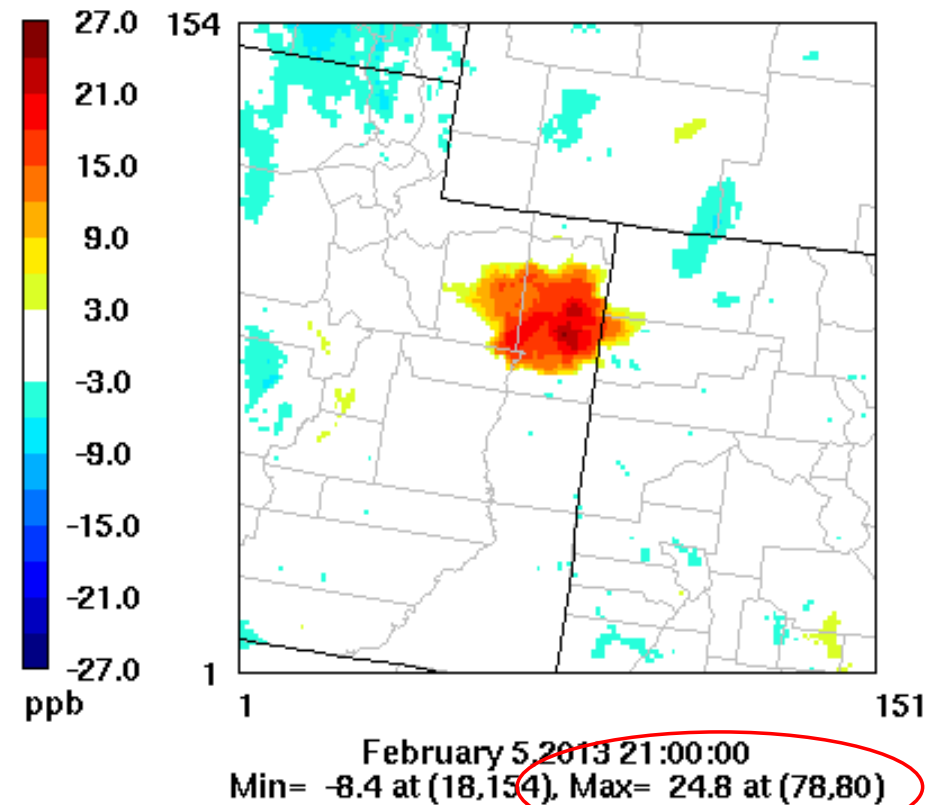
O3 observation sites in the UDAQ 4km



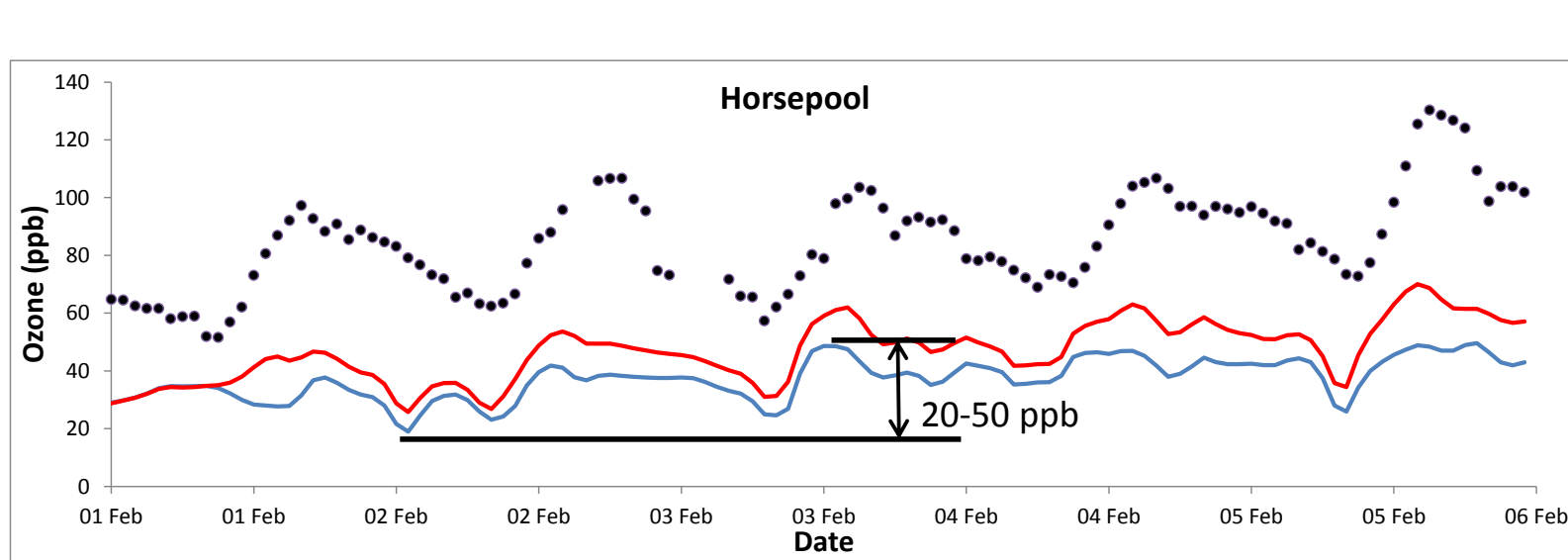
# INITIAL OZONE SIMULATIONS

- Total effect of all model updates:
  - 10-20 ppb O<sub>3</sub> **increase**
- Snow albedo/deposition update:
  - O<sub>3</sub> **increase**
- Winter chemistry update:
  - O<sub>3</sub> **decrease**
- Surface chemistry update re-emitting HONO:
  - O<sub>3</sub> **increase**
  - Surface chemistry configured for **testing purposes only!**
  - Highly speculative, currently no conclusive evidence for a surface chemical pathway

Effect with New Snow + Chemistry Update + Surface Model w/ Snow

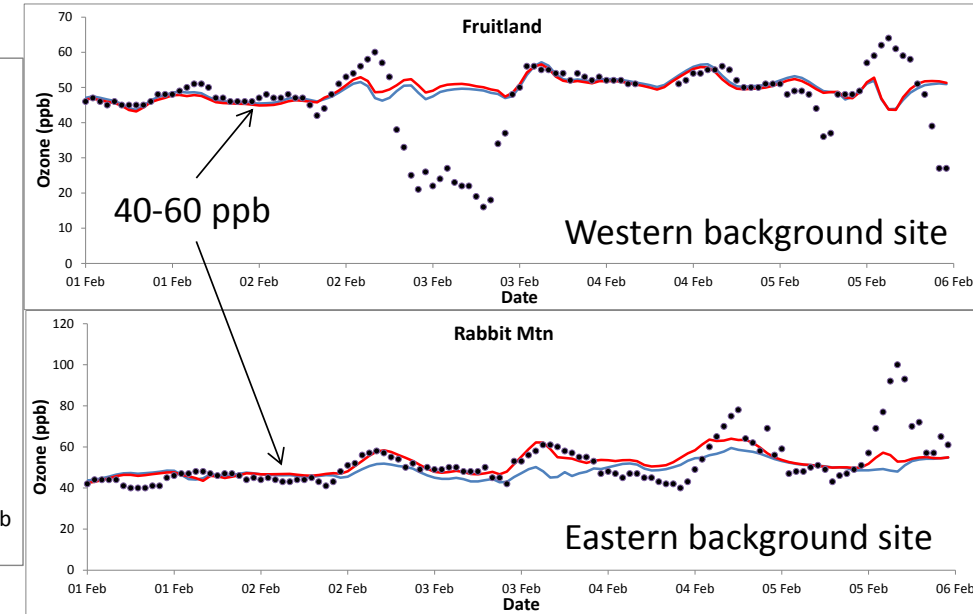


# INITIAL OZONE SIMULATIONS



— Original Model

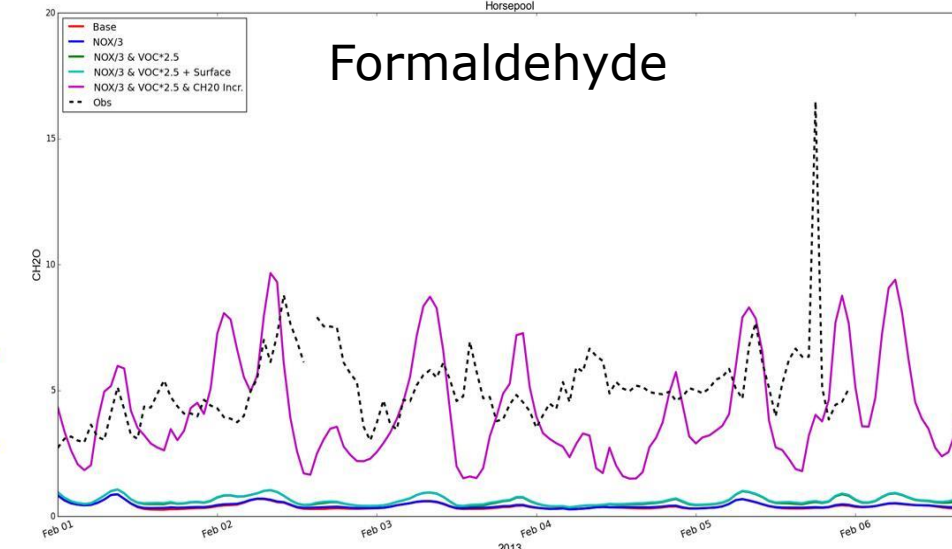
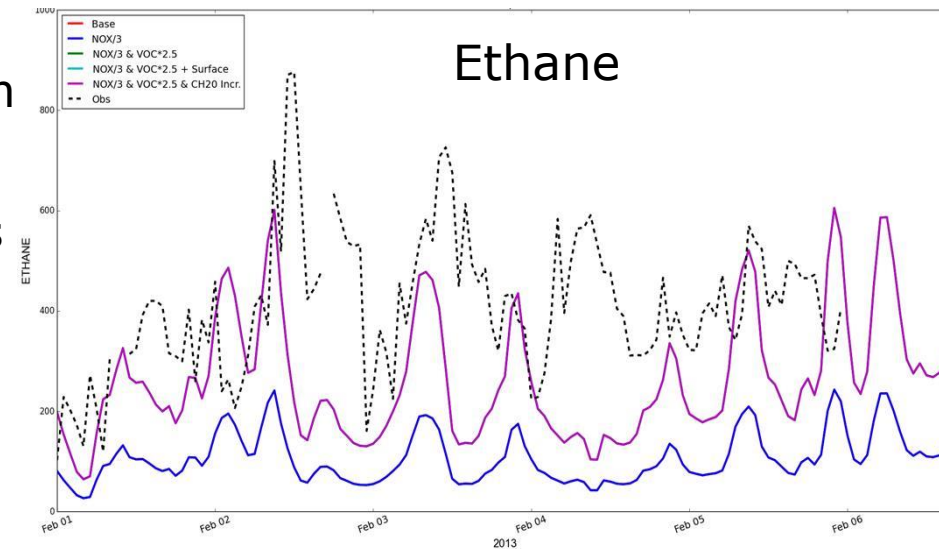
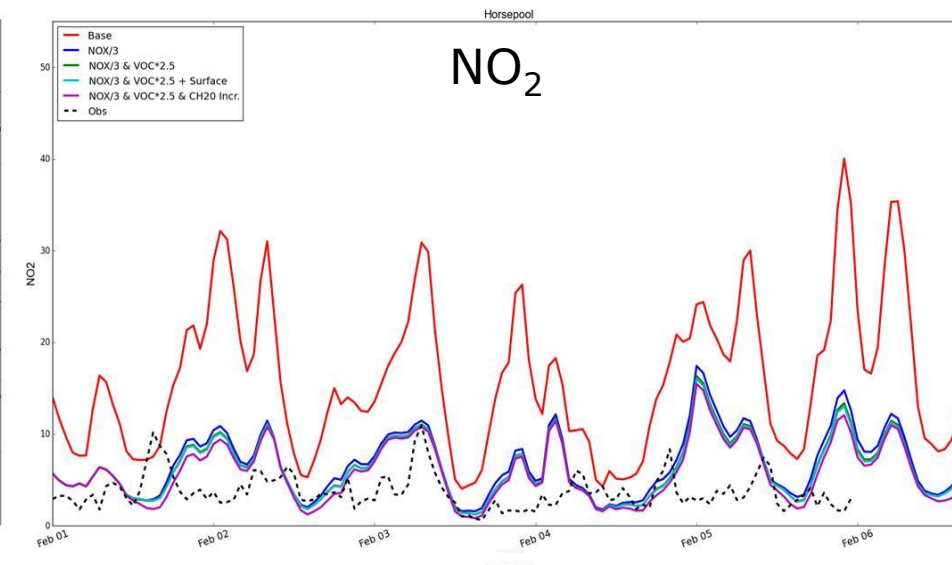
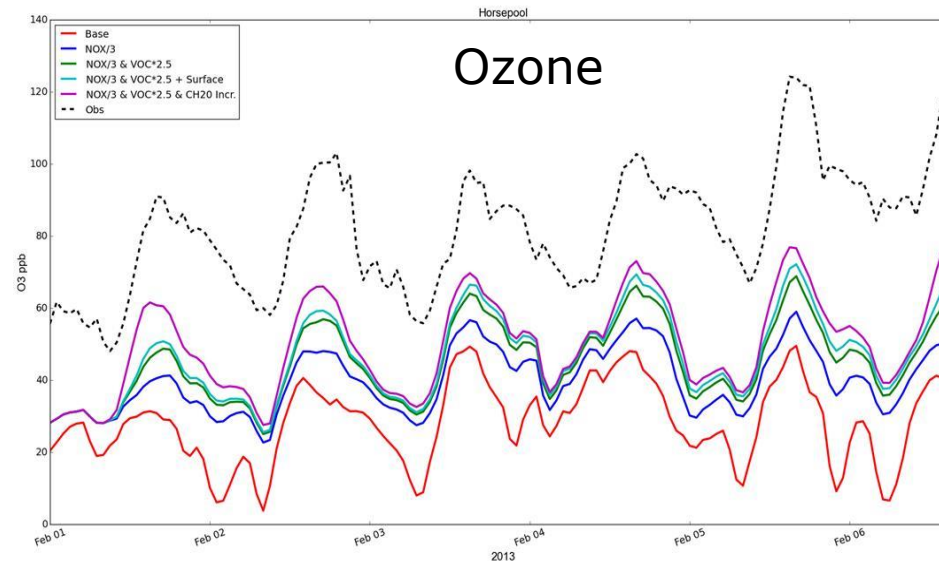
— New snow + Chemistry Update + Surface Model w/ Snow



- $O_3$  is too low in the basin
  - $O_3$  is inhibited and suppressed
  - Comparisons to 2013 UBOS measurements confirm model is  $NO_x$ -rich, VOC-poor
- But background is higher and better simulated outside the basin

# LATEST OZONE SIMULATIONS

- Base (CB6r3+snow)
- NO<sub>x</sub>/3
- NO<sub>x</sub>/3+VOC×2.5
- NO<sub>x</sub>/3+VOC×2.5+Surface Model
- NO<sub>x</sub>/3+VOC×2.5+Formaldehyde
- Still not getting enough ozone
- Ratios of N compounds are wrong – implies missing reactivity



# SUMMARY

- CAMx improvements lead to positive effects, in line with expectations
  - Air chemistry: cold temperatures push NO<sub>x</sub> out of ozone cycle, reduces ozone slightly
  - Snow: higher albedo, reductions in deposition increase ozone
  - Surface/snow chemistry:
    - May be a source of emissions that increase reactivity and ozone production
    - Complex, uncertain, inconclusive – more study needed, but CAMx now has this capability
  - These updates are insufficient to simulate ozone at measured levels
- Need additional work on emission estimates
  - NO<sub>x</sub> oxidation products are not correctly replicated: emission-chemistry cycle is not right
  - Too much NO<sub>x</sub>: over estimated inventory or improper vertical distribution?
  - Too little VOC: under estimating fugitive emissions?
  - Too little formaldehyde: missing a source, ubiquitous use of methanol?



# THANK YOU QUESTIONS?